doi:10.1017/S1431927611007161
Microsc. Microanal. 17 (Suppl 2), 2011

Atomic-scale Interaction Dynamics in Few-layer Hexagonal Boron Nitride (*h*-BN)

Nasim Alem[1,2,3], Quentin Ramasse[4], Michael Sarahan[4], Rolf Erni[5], Oleg V. Yazyev[1,3], Kris Erickson[1,3], Steven G. Louie[1,3], Alex Zettl[1,2,3]

[1] Department of Physics, University of California at Berkeley, Berkeley, California
[2] Center of Integrated Nanomechanical Systems, University of California at Berkeley, Berkeley, California
[3] Materials Sciences Division, Lawrence Berkeley National Laboratory, Berkeley, California
[4] SuperSTEM, STFC Daresbury Laboratories, UK
[5] Empa, Swiss Federal Laboratories for Materials Science and Technology, Switzerland.

Two-dimensional crystals, graphene and hexagonal boron nitride (*h*-BN), consist of a single sheet of sp^2-bonded atoms forming a honeycomb lattice [1]. The atomic structure and surface chemistry of these systems can significantly affect their resulting physical, chemical, and sensing properties. Owing to their large surface area, two-dimensional crystals can interact with various atomic species and functional groups to reduce their surface energy. Such interactions can help with realizing the functionalization of novel sp^2-bonded materials thus changing their physical and chemical properties. For example, the interaction dynamics of graphene with different atomic species reveals the chemical reactivity of this crystal membrane to different functional groups, its energetically favorable sites, and its stability [2-4]. Hexagonal boron nitride is another example of an sp^2-bonded system in which the alternating boron and nitrogen atoms form a polar covalently bonded honeycomb lattice [5, 6]. In contrast to graphene, little work has been done to fully understand the interaction dynamics between *h*-BN and various atomic species, its chemical stability and its active chemical sites.

In this study, we investigate the structure of h-BN and its interaction dynamics by scanning transmission electron microscopy using the Nion UltraSTEM located at Daresbury laboratory operated at 60 kV. This study shows that the electron knock-on damage process of *h*-BN at 60 kV creates various terraces, step edges, defects, and holes in the *h*-BN membrane. Figure 1 shows the formation of a large terrace in *h*-BN with a large single layer next to a hole. Our investigations show that straight zigzag edges seem to be a more stable configuration, similar to the h-BN damage mechanism observed at 80 kV [5]. Furthermore, vacancies are formed as a result of removing a boron atom from the monolayer (1ML) *h*-BN.

Figure 2 shows another region of *h*-BN with large terraces and step edges which provides bonding sites of other chemical species such as carbon adatoms. A hole can be seen in the upper-left corner of the sample in this image next to a double-layer region of *h*-BN. The straight white lines on *h*-BN in Figure 2 show zigzag chains of carbon adatoms, as identified by electron energy loss spectroscopy. Figure 2a shows zigzag carbon chains at the step edges. Zigzag chains of carbon are also formed within the terraces where there is no step edge or defect present (Fig. 2b). Consecutive scans from the region in Figure 2b indicate the movement of the carbon front on the *h*-BN surface, while maintaining its the zigzag configuration. The interactions between *h*-BN lattice and carbon are believed to be surface energy-driven and are further addressed in this study.

References:

[1] K. S. Novoselov et al., *Proceedings of the national academy of sciences of the United States of America,* 102 (2005) 10451.

[2] Gomez-Navarro C, et al., *Nano Letters*, 10 (2010) 1144.
[3] K. Erickson et al., *Advanced Materials*, 22 (2010) 4467.
[4] R. Erni, et al., *Physical Review B*, 82 (2010) 165443.
[5] N. Alem et al., *Physical Review B*, 80 (2009) 155425.
[6] O. L. Krivanek et al., *Nature*, 464 (2010) 571.

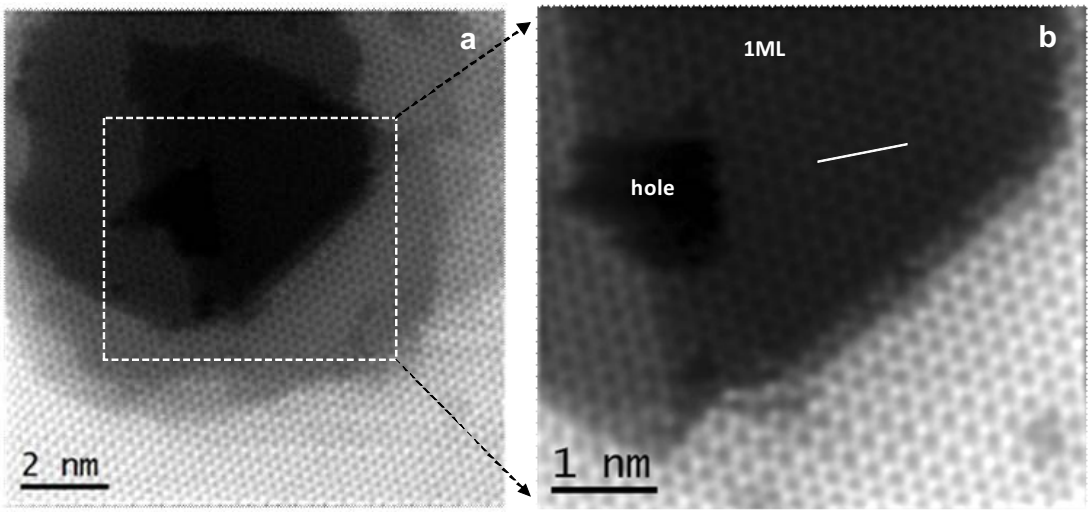
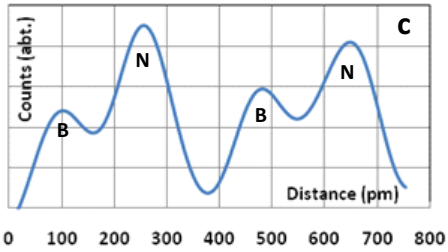


Figure 1. (a) *h*-BN with a few terraces and step edges. (b) A monolayer area of *h*-BN next to a hole. (c) The line profile of the unit cell in the monolayer area indicating nitrogen atoms located on the right side of the unit cell.



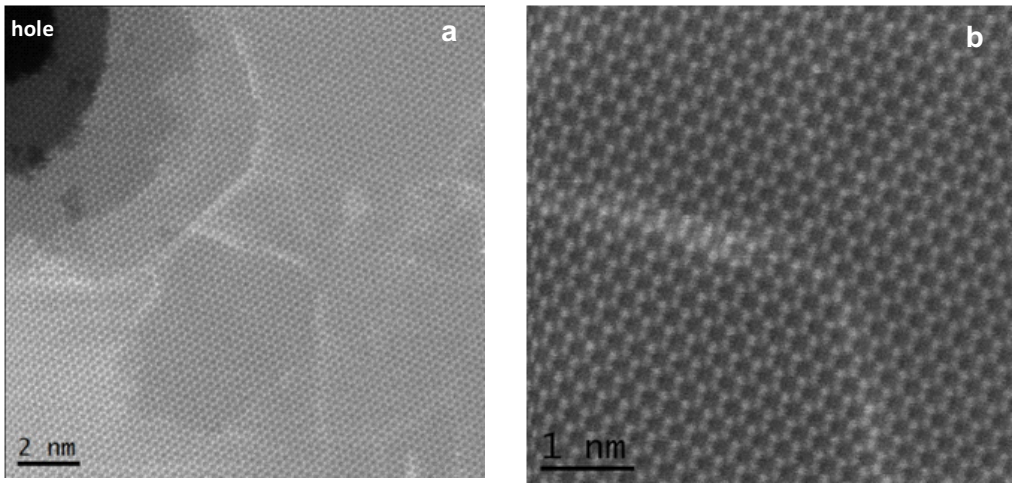


Figure 2. (a) Terraces on *h*-BN created under the electron beam. The bright straight lines show carbon adatoms at the step edges of *h*-BN. (b) A zigzag chain of carbon atoms is observed on the *h*-BN surface, where no step edges or other defects are present.